

Subject: MATERIALS SCIENCE COLLOQUIUM, Peter Zapol, Materials Science Division, Argonne National Laboratory, First Principles Studies of Functional Nanomaterials, Thursday, January 17, 2008, 11:00 a.m., Building 212, Room A-157, Serge Nakhmanson
From: Marlene Metz <metz@anl.gov>
Date: Tue, 08 Jan 2008 10:25:39 -0600
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MATERIALS SCIENCE COLLOQUIUM

SPEAKER: Peter Zapol
Materials Science Division
Argonne National Laboratory

TITLE: "First Principles Studies of Functional Nanomaterials"

DATE: Thursday, January 17, 2008

TIME: 11:00 a.m.

PLACE: Building 212, Room A-157

HOST: Serge Nakhmanson

Refreshments will be available at 10:45 a.m

Abstract:

Computational studies can improve the materials discovery process and have a major impact on science and engineering. This is especially important since new materials underpin fundamental studies of current science drivers such as catalysts, biomaterials, and photovoltaics. Computational design of nanomaterials based on first principles electronic structure calculations is discussed for creating carbon nanotube architectures, optimizing metal and oxide nanoparticle shapes and designing new oxide heterostructures. In particular, three topics will be discussed. Control of carbon dimer adsorption can dramatically modify electronic and phonon properties of nanotubes. Metal nanoparticle shape can be systematically varied by changing their chemical environment during annealing and lead to development of new catalysts. Close proximity of interfaces between oxides of zirconium and indium might lead to new electronic and ionic states affecting charge transport. Given the high cost of experiments, computer simulations emerge as a revolutionary tool for new materials design.

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